Project AD-1689-A

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NONEQUILIBRIUM GASDYNAMICS RELATED TO PROPULSION SYSTEMS

Contract NASr-109
QUARTERLY REPORT for period ending
31 December 1964

1. INTRODUCTION

During the past quarter the research performed under Nonequilibrium Gasdynamics, Contract NASr-109, has concentrated on the following areas:

(1) Preparation of a report on the machine computer code for the numerical solution of the inviscid streamtube flow of a reacting mixture,

(2) Study of impurity effects on vibrational relaxation of nitrogen, using the spectrum line reversal method,

(3) Further development of the technique of spectroscopically following atomic concentrations in shock-wave flows, and

(4) Theoretical studies of vibrational nonequilibrium and vibration-recombination coupling in nozzle-expansion flows.

2. STREAMTUBE PROGRAM REPORT

In the previous quarter work on publishing a report on the CAL computer program for the numerical solution of the inviscid streamtube flow of a reacting mixture was initiated. The following items to be

included in this report were described in the last progress report:

(1) A summary of the governing equations and the methods employed in their solution,

(2) Flow diagrams to illustrate the functions performed by various parts of the computer program,

(3) Detailed listings of the coded computer program (in Fortran),

(4) Instructions for preparation of input data for a general gas model (including specific examples to demonstrate clearly the full capability of the program),

(5) Examples taken from the solutions obtained in the nonequilibrium flow studies mentioned above.

During the past quarter the effort on the writing of the report has been concentrated on items (1) and (2). The section describing the governing equations, in the form used in the computer program, is near completion. Also, the preparation of flow diagrams for the more complicated subroutines has been started. Furthermore, the revision of parts of the program which are unclear has essentially been completed. The recent revisions have involved program changes to eliminate unnecessary error message print-out which occurs in the newer generation of IBM machines (specifically for the 7044 system employed at CAL). In the original version of the program, which was written for the 704, these modifications were not needed.

3. SPECTRUM-LINE REVERSAL STUDIES

Experiments have been initiated to investigate the effect of impurities on the vibrational relaxation of N_2 in a supersonic expansion flow.

The experimental technique utilizes the line-reversal method to monitor the vibrational temperature at a fixed location in the nozzle for constant reservoir conditions. Trace impurities in the form of C_2H_2 (and perhaps O_2 and water vapor) will be added to the test gas in the shock tube and the effect assessed in terms of variations of the observed reversal temperature in the nozzle.

In order to obtain some qualitative indications of the chemical content of the test gas, the emission spectrum of the gas behind the reflected shock wave has been photographed with a small-dispersion prism spectrograph. Spectrograms obtained without the addition of any impurity were found to contain atomic lines almost exclusively. The most predominant atomic line observed was that of the Na-O doublet which is undoubtedly due to residual Na in the shock tube and loading system from previous reversal measurements. The almost complete absence of molecular bands in the pure test gas makes it possible to monitor the reflected shock region for the appearance of molecular impurities. Wavelength calibration of the photographic plate has been obtained by using mercury, cadmium, and Na lamps.

The line-reversal apparatus has been realigned and re-calibrated. A series of measurements are currently being made in pure N_2 expansion flows to insure that the observed temperatures are consistent with earlier results. Initial results indicate complete agreement with the earlier data and provide the basic flow data for the studies of the effects of impurities on the vibrational relaxation. From these runs, a convenient set of reservoir conditions of about 4200°K and 50 atm pressure have been selected for

the basic studies.

It is anticipated that these calibration-type runs will be concluded in the near future and the studies of impurity effects initiated.

4. ATOMIC SPECTROPHOTOMETRIC STUDIES

Assembly is nearing completion of the integrated shock tube-spectrophotometric system which includes the recently completed CAL high-purity shock tube. Vacuum testing of part of the system has already begun. Fabrication of the modified Lyman-α detection system is in process. This will involve reflection of the attenuated Lyman-α signal from a phosphor-coated mirror to a dry-ice-cooled photomultiplier. The original system employed a phosphor coating on the photomultiplier itself, which was at room temperature. The reflectance procedure will increase the gain while the cooling will improve the signal-to-noise ratio by many hundreds of a percent.

It is anticipated that final testing will be accomplished during the last quarter and that the measurements made with the original apparatus will be repeated. The studies will then be extended to other conditions and to observations of the effect of foreign gases.

5. VIBRATIONAL NONEQUILIBRIUM AND VIBRATION-RECOMBINATION COUPLING STUDIES

Under Contract NASr-119 the influence of vibrational relaxation on the rate of dissociation behind shock waves has been investigated.[1,2] Recently, a study has been initiated under the present contract to adapt the theoretical models and computational methods developed in the shock-wave investigation to the case of nozzle-expansion flows. In part, this investigation is being undertaken in an attempt to explain the unexpectedly short relaxation times

observed in recent experimental studies of expanding flows of nitrogen.[3,4] The main long-range purpose of the work is to provide a guide to future experimental studies which will be increasingly concerned with flow situations in which coupling between vibration and dissociation or recombination plays a significant role.

The method employed in studying vibrational relaxation effects on expanding flows is to adapt the computer program for chemical nonequilibrium[5] to this case. In using this method, each vibrational level is treated as a separate chemical species. The collisional de-excitation of vibration can then be written as a unimolecular chemical reaction for each level. In this manner, departures from a Boltzmann distribution of vibrational populations may be accounted for in these situations.

Due to the large number of levels in N_2 and O_2 the size of the kinetic model for vibrational nonequilibrium calculations would be overwhelming, even when dissociation is not included. Consequently, models for the relaxation process which reduce the number of vibrational levels have been examined. The model presently favored assumes the levels to be equally spaced but degenerate. In this way, the real level spacing is represented by varying the degeneracy of the levels in the model oscillator. The work on establishing a model for the vibrational mode closely parallels the studies for shock wave flows under Contract NASr-119.

The initial work in this area has been concentrated on flows of nitrogen and oxygen heavily diluted with argon. By studying dilute mixtures, only the vibrational de-excitation and recombination paths involving argon as a collision partner need be considered. This further reduces the number of

reactions to be considered.

A model has been formulated and preliminary results obtained for vibrational relaxation in nitrogen-argon mixtures. In these calculations the de-excitation rates are assumed to increase with level number due to the change in the frequency of the level. No dissociation is included and the calculations are aimed at deciding on an appropriate frequency dependence for the vibrational de-excitation rates. The decision will be based on comparison of the calculated results with experimental results from both shock wave and nozzle flow measurements.

Once the vibrational de-excitation part of the model has been formulated calculations for oxygen-argon and nitrogen-argon nozzle flows including recombination will be carried out. It is planned to concentrate on studies of dilute mixtures in the remainder of the present contract period.

REFERENCES

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3. Hurle, I. R., Russo, A. L. and Hall, J. G., "Spectroscopic Studies of Vibrational Nonequilibrium in Supersonic Nozzle Flows". J. Chem. Phys. 40, 2076 (1964).

4. Hurle, I. R. and Russo, A. L., "Spectrum-Line Reversal Measurements of Na Excitation in Ar and N_2-Ar Expansion Flows Containing Free Electrons". To be submitted to J. Chem. Phys.

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